Semi-Markov Random Walks and Universality in Ising-like Chains.

M. Droz
Département de Physique Théorique
Université de Genève CH-1211 Genève 4
and
M.-O. Hongler
Département de Microtechnique
Institut de Production Microtechnique *
Ecole Polytechnique Fédérale de Lausanne

February 1, 2008

CH-1015 Lausanne

Abstract

We exhibit a one to one correspondence between some universal probabilistic properties of the ordering coordinate of one-dimensional Ising-like models and a class of continuous time random walks. This correspondence provides an new qualitative picture of the properties of the ordering coordinate of the Ising model.

1 Introduction

Many systems in Nature exhibit a phase transition when a control parameter (the reduced temperature for example) ϵ is varied. Often, the phase transition is related to a spontaneous symmetry breaking in the system: one phase is less symmetric than the other, and the so-called order parameter ϕ describes this symmetry breaking. The parameter ϕ could be a scalar, a vector or a tensor and its number of components n is an important parameter.

The amplitude of the order parameter is zero in the most symmetric phase and nonzero in the less symmetric one. If the order parameter varies continuously at the transition, one speaks of a second order phase transition. It turns out that, near a second order transition point, every physical quantity \mathcal{A} (like the specific heat, the susceptibility, ...) can be written as the sum of a regular part and a singular one in ϵ . The singular part (\mathcal{A}_s) behaves as power law $\mathcal{A}_s \sim |\epsilon|^{-\alpha}$ providing that the control parameter ϵ has been chosen as to vanish at the critical point. The parameter α is called the "critical exponent" associated to \mathcal{A} .

A remarquable feature of second order phase transitions is the so-called "universality". Scaling theory [1] and renormalization group arguments [2] show that, the critical

^{*}Dirigé par le Professeur Jacques Jacot

exponents are only function of n and d, the dimensionality of the system. Thus systems as different as for example an Ising model (describing the paramagnetic ferromagnetic transition in one component spin system) and a model of a fluid (describing the liquid gas transition) belong to the same universality class.

A less investigated problem concerns the universal aspect of ordering coordinate underlying critical point singularities. A. Bruce [3] has investigated this problem in the case of an Ising-like problem, i.e. a problem for which the scalar order parameter is the ensemble average of a one-component local spin variable $\sigma(x)$. The configurational energy consists of local double well potentials and the short-range interaction among the spins. Each stochastic variable $\sigma(x)$ is characterized by its probability density distribution $P(\sigma)$. This function has a whole spectrum of possible forms, but two extreme cases can be singularized. At low temperature, the thermal energy is much smaller than the depth of the potential wells. Thus the ordering coordinate are localized in the vicinity of the two well minima and $P(\sigma)$ has a strongly two-peaked form. One speaks of the "ordered" limit. Alternatively, at high temperature, the potential wells are so shallow that the local coordinate is nearly distributed about the symmetric state $\sigma=0$. One speaks of the "disordered" limit.

Parallel to the spin system, the continuous time random walks, (also called randomized random walks in W. Feller, [4]), do play an important role in the modeling of transport phenomena in disordered media, (see [5], for a recent bibliography on this topic). Firm mathematical basis to describe this class of processes, can be found in [6] and [7], the later being more directly related to one aspect of the models to be described here. The simplest situation consists of a symmetric random walks on the infinite one-dimensional, (1-D), lattice with lattice spacing a and with the random time between consecutive the jumps being exponentially distributed. In this case, the position of the walker is described by a markovian Master Equation. When the time between the jumps is drawn from non-exponential distributions, non-markovian properties arise and to describe these situations E. Montroll and G. Weiss proposed a generalization of the Master equation [8]. In the present paper, we shall consider the non-markovian random walks obtained when the time intervals between jumps are drawn from generalized Erlang distributions. These distributions defined on $[0,\infty]$ belong to the general class of phase-type distributions which describe the time until absorption of a finite state continuous time Markov chain [9]. For this class of random processes, we shall observe that, when large time are considered, the probablistic properties of the position of the walker exhibit a universal behavior which is in one to one correspondence with the probabilistic properties of the ordering coordinates of a one-dimensional Ising spin systems.

Our paper is organized as follows in section 2, a brief account of the universal properties of Ising-like systems are given. In particular, the probability distribution of a collective coordinates in an Ising chain is recalled. In section 3, we introduce the relevant class of continuous time random walks to be used and calculate the probability density describing the position of the walker. In the last section, we exhibit the one to one correspondence which can be drawn between the two classes of models.

2 Universal properties of the probability density distribution of the collective coordinates in Isinglike models.

Let us return to the Ising-like system described in the introduction. To be able to detect the universal features of the ordering coordinates, one has then to coarse-grained

the problem and considers "bloc-spin" variables $\sigma_L(x)$ representing the effective spin of a block of linear size L. The variable σ_L is also a random variable characterized by its probability density distribution $P(\sigma_L, L)$. Renormalization group arguments suggest that $P_L(\sigma_L, L)$ tends to an universal limiting form P^* when both L and the correlation length ξ are much larger than a, the lattice spacing. It turns out that in one dimension the probability density function P^* can be computed exactly using a matrix transfert operator technique [3]. Furthermore, the critical temperature of one-dimensional Ising-like systems with short range interactions is zero. The low temperature properties of the block coordinate probability distribution function, for large block size, is governed by the statistical mechanics of the cluster walls [10]. Thus to compute $P(\sigma_L, L)$ for our one-dimensional Ising like models, it suffices [3] to consider a one dimensional fixed-length spin Ising model, $\sigma(x_i) = \pm \sigma_0$, with nearest neighbors interactions and the following effective Hamiltonian (in units of $k_B T$, where k_B is the Boltzmann constant and T the temperature):

$$\mathcal{E} = -\frac{K}{\sigma_0^2} \sum_{i=1}^{N} \sigma(x_i) \sigma(x_{i+1}) \tag{1}$$

 σ_0 is chosen such as $P(\sigma_L, L)$ has an unit variance.

It is known [11] that (in the thermodynamic limit $N \to \infty$) the two-point correlation function of this model is:

$$C_2(r) = \langle \sigma(x)\sigma(x+r) \rangle = \sigma_0^2 \left[\tanh(K) \right]^r = \sigma_0^2 \exp(-r/\xi)$$
 (2)

where

$$\xi = \frac{1}{2} \exp(2K)[1 + \mathcal{O}(\exp(-4K))] \tag{3}$$

is the correlation length.

The block coordinate takes the simple form

$$\sigma_L = \frac{1}{L\sigma_0} \sum_{i=1}^{L} \sigma(x_i). \tag{4}$$

To compute $P(\sigma_L, L)$ it is suitable to introduce its Fourier transform $\tilde{P}(H, L)$:

$$P(\sigma_L, L) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \tilde{P}(H, L) \exp(-iH\sigma_L) dH, \tag{5}$$

 $\tilde{P}(H,L)$ is simply the characteristic function from which the n-point cumulants can be derived. Moreover, $\tilde{P}(H,L)$ can also be written as [3]:

$$\tilde{P}(H,L) = \frac{Z(iH)}{Z(0)},\tag{6}$$

where Z(h) is the canonical partition function defined as

$$Z(h) = Tr_{\{\sigma(x_i)\}} \exp\left[-\mathcal{E} + \frac{h}{L\sigma_0} \sum_{i=1}^{N} \sigma(x_i)\right]. \tag{7}$$

The traces Z(h) and Z(0) can be readily computed by the usual transfert matrix method [11] for h real. The analytic continuation to the imaginary h axe is unique.

In the large L and ξ regime, one finds [3] that $\tilde{P}(H,L)$ is indeed an universal function, denoted $\tilde{P}^*(H,z)$, depending only upon the reduced variable $z=L/\xi$:

$$\tilde{P}^*(H,z) = \exp(-\frac{z}{2}) \left\{ \cosh\left(\sqrt{\frac{z^2}{4} - H^2}\right) + \frac{1}{\sqrt{1 - \frac{4H^2}{z^2}}} \sinh\left(\sqrt{\frac{z^2}{4} - H^2}\right) \right\}. \tag{8}$$

By inverse Fourier transform one finds:

$$P^*(\sigma_L, z) = \frac{1}{2} \exp(-\frac{z}{2}) \left\{ \left(\delta(1 - \sigma_L) + \delta(1 + \sigma_L) \right) \right\} + \frac{z}{4} \exp(-\frac{z}{2}) \left[I_0 \left(\frac{z}{2} (1 - \sigma_L^2)^{1/2} \right) + \frac{I_1 \left(\frac{z}{2} (1 - \sigma_L^2)^{1/2} \right)}{(1 - \sigma_L^2)^{1/2}} \right] \Theta(1 - \sigma_L^2).$$
 (9)

Two particular limits deserve a special attention:

• i). The critical limit: $z \to 0$. In this case one finds:

$$P^*(\sigma_L, z) \approx \frac{1}{2} \Big[\delta(1 - \sigma_L) + \delta(1 + \sigma_L) \Big]. \tag{10}$$

Hence the probability distribution function has a limiting "ordered" form.

• ii). The non-critical limit: $z \to \infty$. In this cas, one finds

$$P^*(\sigma_L, z) \approx \sqrt{\frac{z}{4\pi}} \exp\left(\frac{-z\sigma_L^2}{4}\right)$$
 (11)

which corresponds to the "disordered" limit.

3 Semi-Markov Birth and Death processes

Now we consider a symmetric birth and death process on the infinite 1-D lattice: $\mathbf{Z}_a=\{...,-a,0,+a,2a,...\}$, a being the lattice spacing. The jumps of the random walker occur at random times $\xi_0,\,\xi_1,\,\xi_2$ and the interval of time between successive jumps is denoted $\tau_k=\xi_{k+1}-\xi_k$, $k=0,\,1,\,2,...$. We assume the τ_k to be independent and identically distributed random variables. Let $\psi(\vec{\lambda},\vec{\mu},t)$ be the probability density from which the $\{\tau_k\}$'s are drawn. The constant vectors $\vec{\lambda}=\{\lambda_0,\lambda_1,....\lambda_N\}$ and $\vec{\mu}=\{\mu_0,\mu_1,...\mu_M\}$ are parameters characterizing the distributions of the time between consecutive jumps. Accordingly, we shall write:

$$\operatorname{Prob}\left\{t \le \tau \le t + dt\right\} = \psi(\vec{\lambda}, \vec{\mu}, t)dt. \tag{12}$$

From now on, we shall assume that $\psi(\vec{\lambda}, \vec{\mu}, t)$ is called a PH-Type density, which can be defined by its Laplace transform:

$$\int_0^\infty \psi(\vec{\lambda}, \vec{\mu}, t) e^{-ut} dt = \widetilde{\psi}(\vec{\lambda}, \vec{\mu}, u) = \frac{\Pi_{\vec{\mu}}}{\Pi_{\vec{\lambda}}}$$
 (13)

with the definitions:

$$\Pi_{\vec{\lambda}} = \begin{cases}
\Pi_{k=1}^{N} (1 + \frac{u}{\lambda_{k}}), & \text{for } N \ge 1, \\
1, & \text{for } N = 0.
\end{cases}$$
(14)

and

$$\Pi_{\vec{\mu}} = \begin{cases}
\Pi_{k=1}^{M} (1 + \frac{u}{\mu_{k}}), & \text{for } M \ge 1, \\
1, & \text{for } M = 0.
\end{cases}$$
(15)

We impose that N > M. In view of Eqs.(13), (14) and (15), we immediately obtain:

$$\langle \tau \rangle = -\frac{\partial}{\partial u} \widetilde{\psi}(\vec{\lambda}, \vec{\mu}, u) \mid_{u=0} = \sum_{k=0}^{N} \frac{1}{\lambda_k} - \sum_{k=0}^{M} \frac{1}{\mu_k} > 0, \tag{16}$$

and the variance of the time between consecutive jumps reads as:

$$\sigma_{\tau}^{2} = \langle \tau^{2} \rangle - \langle \tau \rangle^{2} = \frac{\partial^{2}}{\partial u^{2}} \widetilde{\psi}(\vec{\lambda}, \vec{\mu}, u) \mid_{u=0} - \left[-\frac{\partial}{\partial u} \widetilde{\psi}(\vec{\lambda}, \vec{\mu}, u) \mid_{u=0} \right]^{2} = \left[\sum_{k=1}^{N} \frac{1}{\lambda_{k}} \right]^{2} - \sum_{k \neq m}^{N} \frac{1}{\lambda_{k} \lambda_{m}} - \left[\sum_{k=1}^{M} \frac{1}{\mu_{k}} \right]^{2} + \sum_{k \neq m}^{M} \frac{1}{\mu_{k} \mu_{m}}.$$

$$(17)$$

Let us now return to our random walk and denote by P(sa,t) the probability to find the walker at the position sa at time t. We shall assume:

$$P(sa, 0) = \delta_{sa,0}$$
 and $\xi_0 = 0$. (18)

where $\delta_{sa,0}$ is the Kronecker symbol. Using the formalism introduced in [5] and [6], it is shown in [12] that P(sa,t) obeys to the high order differential difference equation:

$$\prod_{k=0}^{N} (1 + \frac{1}{\lambda_k} \frac{\partial}{\partial t}) P(sa, t) = \prod_{k=0}^{M} (1 + \frac{1}{\mu_k} \frac{\partial}{\partial t}) \left[P((s+1)a, t) + P((s-1)a, t) \right]. \tag{19}$$

To solve Eq.(19), we would need to specify the appropriate initial conditions, $\frac{\partial^m}{\partial t^m}P(sa,t)|_{t=0}$ for m=1,2,...,N-1. As we shall not derive, in this paper, solutions of Eq.(19), we refrain to give here further details on the characterization of these initial conditions. Let us now give two simple illustrations:

• Example 1: With N=1 and M=0, Eq.(19) takes the form:

$$\left(1 + \frac{1}{\lambda_0} \frac{\partial}{\partial t}\right) P(sa, t) = \frac{1}{2} \left[P\left((s+1)a, t\right) + P\left((s-1)a, t\right)\right]$$
(20)

which is the Master equation for the continuous time Markov random walk.

• Example 2: With $N=2, \lambda_0=\lambda_1$ and M=0, Eq.(19) takes the form:

$$\left(\frac{\partial^2}{\partial t^2}P(sa,t) + 2\lambda_0 \frac{\partial}{\partial t}P(sa,t)\right)P(sa,t) =$$

$$\lambda_0^2 \left[-P(sa,t) + \frac{1}{2}P\left((s+1)a,t\right) + \frac{1}{2}P\left((s-1)a,t\right) \right]$$
(21)

with the initial condition being for this case: $\frac{\partial}{\partial t}P(sa,t)|_{t=0}$.

For small lattice spacing a, we expand the right hand side of Eq.(19) up to second order in a:

$$\prod_{k=1}^{N} \left(1 + \frac{1}{\lambda_k} \frac{\partial}{\partial t} \right) P(x, t) = \prod_{k=1}^{M} \left(1 + \frac{1}{\mu_k} \frac{\partial}{\partial t} \right) \left[P(x, t) + \frac{a^2}{2} \frac{\partial^2}{\partial x^2} P(x, t) \right]$$
(22)

where we have written $sa = x \in \mathcal{R}$. As usual, we now rescale the time variable as:

$$T = a^2 t. (23)$$

Introducing Eq.(23) into Eq.(22), we obtain:

$$\sum_{k>2}^{N} C_k a^{2k} \frac{\partial^k}{\partial T^k} P(x,T) + a^4 C_2 \frac{\partial^2}{\partial T^2} P(x,T) + a^2 C_1 \frac{\partial}{\partial T} P(x,T) =$$

$$\frac{a^2}{2} \frac{\partial^2}{\partial x^2} P(x, T) + \sum_{k>1}^M a^{2k+2} \mathcal{B}_k \frac{\partial^k}{\partial T^k} \frac{\partial^2}{\partial x^2} P(x, T), \tag{24}$$

where C_k and B_k are constant coefficients $\forall k$. Using Eq.(16), we have in particular:

$$C_1 = \langle \tau \rangle. \tag{25}$$

When M=0, the PH-Type distribution Eq.(13) reduces to the E_n-type distribution, (generalized Erlang distributions of order n). From now on, we shall focus our attention to this class of E_n-type models. Retaining the terms up to order a^2 in Eq.(24), we have therefore when M=0:

$$a^{2}C_{2}\frac{\partial^{2}}{\partial T^{2}}P^{*}(x,T) + \langle \tau \rangle \frac{\partial}{\partial T}P^{*}(x,T) = \frac{1}{2}\frac{\partial^{2}}{\partial x^{2}}P^{*}(x,T). \tag{26}$$

where the superscript * for $P^*(x,T)$ indicates that we restrict ourselves to the E_n -type model. In view of Eqs. (24), (16) and (17), we can write:

$$C_2 = \frac{1}{2} \left(\langle \tau \rangle^2 - \sigma_\tau^2 \right) = \frac{1}{2} \langle \tau \rangle^2 \left(1 - CV_\tau^2 \right)$$
 (27)

where CV_{τ}^2 stands for the coefficient of variation which for E_n -type distribution is always smaller than unity.

Eq.(26) is the celebrated Telegrapher's equation which, in the asymptotic regime, appears as a "universal" description for all random walks with time between the jumps drawn from E_n -type distributions.

Introducing the Fourier transform:

$$\tilde{P}^*(k,T) = \int_0^\infty P^*(x,T) e^{-ikx} dx,$$
 (28)

the Telegrapher's Eq.(26) takes the form:

$$a^{2}C_{2}\frac{\partial^{2}}{\partial T^{2}}P^{*}(k,T) + \langle \tau \rangle \frac{\partial}{\partial T}P^{*}(k,T) = \frac{k^{2}}{2}P^{*}(k,T)$$
(29)

and the solution of Eq.(29) with initial conditions:

$$\widetilde{P}^*(k, T=0) = 0$$
 and $\frac{\partial}{\partial T}\widetilde{P}^*(k, T)|_{T=0} = 0$ (30)

reads immediately as in Eq.(8), provided we reinterpret the parameters as:

$$z = \frac{2T}{g\langle \tau \rangle a^2} \quad \text{and} \quad H^2 = \frac{qa^2}{4} z^2 k^2, \tag{31}$$

with

$$q = (1 - CV_{\tau}^2) \in [0, 1].$$
 (32)

By direct inversion, the density Eq.(9) follows provided we introduce the identification:

$$\sigma_L^2 = \frac{4x^2}{z^2 a^2 q}. (33)$$

Although this is not necessary, we can chose T = 1 which corresponds to the definite scale factor chosen in [3], (see Eq. (2.11) in A. Bruce, [3]).

Hence, the critical and non critical regimes described by Eq.(10) and (11) follows directly.

4 Conclusion

The Telegrapher's equation Eq.(26) and its solution Eq.(9) describe the asymptotic behavior of the probability density for both the coarse-grained variables of an Ising-like chain and the position of continuous time random walker.

The behavior of the block coordinate of the Ising system is similar to the behavior of a random walker with time between the jumps drawn from an E_n type distribution. This can be understood qualitatively as follows: consider the coarse-grained variable of the Ising model including a given, (large), number of spins, say N >> 1. Add one spin to this sample of N spins and consider the new probability density distribution of the block spin coordinate. Two main factors influence the result:

- 1) the correlation between nearest-neighbor spins.
- 2) the fact that in the large sample N limit, only the spins with values close to $\pm \sigma_0$ will contribute to the coarse-grained variables.

Hence, to an increase of the sample used to construct the coarse-grained spin variable in the Ising model corresponds an increase of the time in the continuous time random walk with a lattice sapcing being related to σ_0 . Furthermore, the "aging" effect implied by the use of non-exponential distributions for the time intervals between the jumps directly describes the correlation between the spin variables in the Ising model. Quantitatively, the roles played by the parameters of the two models are as follows: to the parameter $\tanh(K) \in [0,1], K \geq 0$ defined in Eq.(2), we can directly associate the parameter $q \in [0,1]$ defined in Eq.(32). This correspondence is physically consistent as $\tanh(K)$ measures the correlation between nearest-neighbor spin variables given by Eq.(2) while q relates the memory effects of the semi-markovian random walk. Two limiting regimes deserve attention:

- a) Weak correlation regime. Here $q \to 0 \Leftrightarrow CV_{\tau}^2 = 1$ and hence $\tanh(K) \Leftrightarrow 0 \Rightarrow K \to 0$. We then reach here the markovian regime of the random walk. Accordingly, the $z \to \infty$ limit arises in Eq.(31) which implies an absence of correlations between the spins.
- b) Strong correlation regime. To the limit $K \to \infty \Rightarrow \tanh(K) \to 1$ corresponds the $q = 1 \Rightarrow CV_{\tau}^2 = 0$ regime for the continuous time random walk. As $CV_{\tau}^2 = 0$, the time intervals between the jumps become equally spaced and this therefore corresponds to a discrete, (deterministic), time random walk. Accordingly, we have $z \to 0$ and therefore the double-peak shape of the probability density exhibited in Eq.(10) arises consistently.

Acknowledgments

MD is partially supported by the Swiss National Science Foundation.

References

- [1] Stanley H.E. 1971 Introduction to Critical Phenomena, (Oxford: Clarendon)
- [2] Ma S.K. 1976 Modern Theory of Critical Phenomena, (Reading, Mass: Benjamin)

- [3] Bruce A. D. "Probability density Functions for Collective coordinates in Ising-Like Systems" 1981 J. Phys. C: Soliod State Phys. 14 3667-3688
- [4] Feller W. An introduction to Probability theory and its applications 1971, Vol. II, (J. Wiley, New-York).
- [5] Hughes B. D. Random Walk and Random Environments 1995, Vol. II, (Clarendon Press, Oxford)
- [6] Cinlar E. "Markov Renewal Theory: A Survey" 1975 Management Science 21, 727-752.
- [7] G. Latouche. "A Phase Type Semi-Markov Point process". 1982 SIAM J. Alg. Disc. Meth. 3, 77-90.
- [8] Montroll E. W. and Weiss G. H. "Random Walks on Lattice II" (1965) J of Math. Phys. 6, 167-181.
- [9] Neuts M. 1981 Matrix Geometric Solutions in Stochastic Models (John Hopkins Press, Baltimore)
- [10] Krumhansl J.A. and Schreiffer J.R. "Dynamics and statistical mechanics of a one-dimensional model Hamiltonian for structural phase transitions" 1975 Phys. Rev. **B11** 3535-3545.
- [11] Thompson C.J. 1972 Mathematical Statistical Mechanics, (Princeton Univ. Press).
- [12] Hongler M.-O. and Salama Y. "Semi-Markov Processes with Phase-Type waiting times" 1996 Zeit. fr Angew. Math. und Mech. (ZAMM) **76** Suppl. 461-462